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Zafer Çıplak, ***Furkan Soysal***, Ceren Atila Dinçer, Aslıhan Öztürk, ***Nuray Çelebi***, Kouroush Salimi, Nuray Yıldız

Parametric study of Z-scheme rGO-Fe3O4-CuO ternary nanocomposites for efficient visible-light-driven organic dye degradation

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Parametric study of Z-scheme rGO–Fe_3O_4–CuO ternary nanocomposites for efficient visible-light-driven organic dye degradation

Zafer Çıplak[a], Furkan Soysal[b], Ceren Atila Dinçer[c], Aslıhan Öztürk[c], Nuray Çelebi[b], Kouroush Salimi[d], and Nuray Yıldız[c]

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ABSTRACT

In this study, magnetic nanocomposites based on reduced graphene oxide (rGO) were synthesized and their photocatalytic activities were investigated. rGO–Fe_3O_4 nanostructures were synthesized by the solvothermal method and copper oxide (CuO) nanoparticles were deposited on the surface at different ratios by the co-precipitation method. Binary and ternary nanocomposites with different component ratios (rGO–Fe_3O_4, rGO–Fe_3O_4–CuO (1:8:0.5, 1:8:1, and 1:8:2)) were characterized by XRD (X-Ray Diffraction), SEM (Scanning Electron Microscope), TEM (Transmission Electron Microscope), UV–Vis (UV–visible Spectrophotometer), and FTIR (Fourier Transform Infrared Spectroscopy). Photocatalytic activity of the prepared nanocomposites was observed with methylene blue (MB) dye under visible LED light. The results showed that the synthesized nanocomposites had photocatalytic efficiencies ranging from 36% to 89% depending on the component ratio. The rational incorporation of CuO into rGO–Fe_3O_4 significantly improved photocatalytic efficiency and demonstrated a stable Z-scheme heterostructure, highlighting the potential of this ternary composite for efficient and scalable wastewater treatment.

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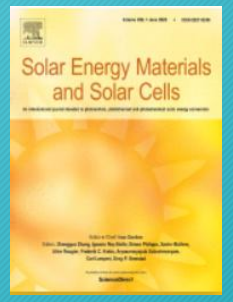
KEYWORDS
Reduced graphene oxide; photocatalytic degradation; nanocomposites; metal oxide nanoparticles

Abid Ustaoglu, Mustafa Sabri Gok, ***Bülent Yeşilata***, Kasım Ozacar, Zeyad Amjed, Tayfun Altiok, Alaattin Metin Kaya, Fatih Kocyigit

Experimental and machine learning investigation of a solar air heater with a novel compact thermal absorber design



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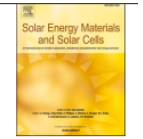

Abid Ustaoglu [a,b,*], Mustafa Sabri Gok [a], Bülent Yeşilata [c], Kasım Ozacar [d], Zeyad Amjed [e], Tayfun Altiok [e,f], Alaattin Metin Kaya [g,h], Fatih Kocyigit [i]

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ARTICLE INFO

Keywords:
Solar air heater
Compact heat exchanger
Thermal–exergy analysis
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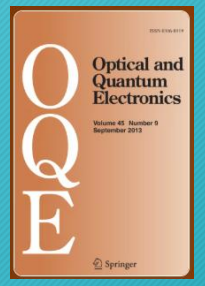
ABSTRACT

This study presents the development and evaluation of a novel and sustainable solar air heater (SAH) incorporating an enhanced compact heat-absorbing structure made from recycled aluminum radiator fins, designed to improve thermal and exergetic-performance while promoting material-reuse and sustainability. The reuse of waste radiator materials provides a multilayered-fin configuration that increases the effective heat-transfer surface area, enhances turbulence, and reduces overall heat loss without additional manufacturing cost. A comparative methodology was employed to assess the influence of this compact thermal-storage element on SAH performance under typical Autumn and Spring conditions. The baseline and modified SAH models were evaluated using dimensionless performance parameters and validated through experimental testing. The average thermal-efficiency of the baseline system was 64.81 %, while the compact heat-exchanger-integrated system reached 78.54 %, indicating a significant improvement of about 13.7 percentage points (21 % relative increase). Furthermore, the oriented-configuration (ochxSAH) provided an additional 3.23 percentage points improvement, corresponding to a further 4 % performance gain. The heat loss rate for chxSAH increase 5.9 % that accompanied a much larger rise in useful heat-gain, confirming improved energy utilization efficiency. These gains were achieved through the improved energy-saving capacity of the recycled radiator-based absorber and its ability to maintain higher outlet temperatures. To complement the experimental study, a machine-learning (ML) approach was applied to predict SAH efficiency. The ML results validated the superior thermal and exergy performance of the sustainable SAH design, demonstrating that integrating waste-material-based compact heat exchangers can enhance system efficiency while supporting circular-economy principles in solar-thermal technologies.

Aisha R Al-Marhabi, Reda M El-Shishtawy, Khalid O Al-Footy, Kenan Ozel, Abdullah Atilgan, ***Abdullah Yildiz***

Donor moiety engineering in D-D-π-A-π-A quinoxaline sensitizers for efficient dye-sensitized solar cells



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Donor moiety engineering in D-D-π-A-π-A quinoxaline sensitizers for efficient dye-sensitized solar cells

Aisha R. Al-Marhabi[1] · Reda M. El-Shishtawy[2,3] · Khalid O. Al-Footy[2] · Kenan Ozel[4] · Abdullah Atilgan[5] · Abdullah Yildiz[6]

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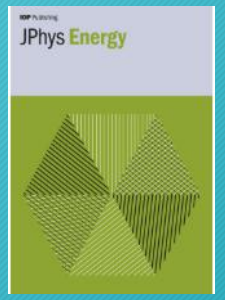
Abstract
Quinoxaline-based organic sensitizers are promising candidates for improving the efficiency of dye-sensitized solar cells (DSSCs) due to their strong electron-withdrawing characteristics and tunable electronic structures. In this study, we investigated the effect of donor moiety engineering on the performance of three D-D-π-A-π-A quinoxaline sensitizers (QX-D1, QX-D2, and QX-D3), incorporating phenothiazine, phenoxazine, and carbazole donors, respectively. Comprehensive optical, electrochemical, and photovoltaic analyses revealed distinct structure–property–performance correlations. Among the three dyes, QX-D3 exhibited the most favorable light-harvesting ability, achieving a power conversion efficiency of 6.45% with a high short-circuit current density of 19.96 mA cm^{-2}. Electrochemical impedance spectroscopy confirmed that QX-D3 provided superior recombination resistance, longer electron lifetimes, and the highest charge collection efficiency. These results highlight the critical role of donor design in enhancing light absorption, charge injection, and suppression of recombination, offering a rational pathway for the molecular engineering of efficient metal-free sensitizers in DSSCs.

Keywords Quinoxaline sensitizers · Phenothiazine · Phenoxazine · Carbazole · Donor, DSSC performance, D-D-π-A-π-A type.

K Ozel, EB Yurdakul, N Akdogan, ABDULLAH Atilgan, HALİT Arslan, ***ABDULLAH Yildiz***, A Disli, Y Erdogdu

Synthesis, photophysical, electrochemical, and quantum chemical investigations of a novel phenothiazine-derived organic dye for high efficiency dye-sensitized solar cells



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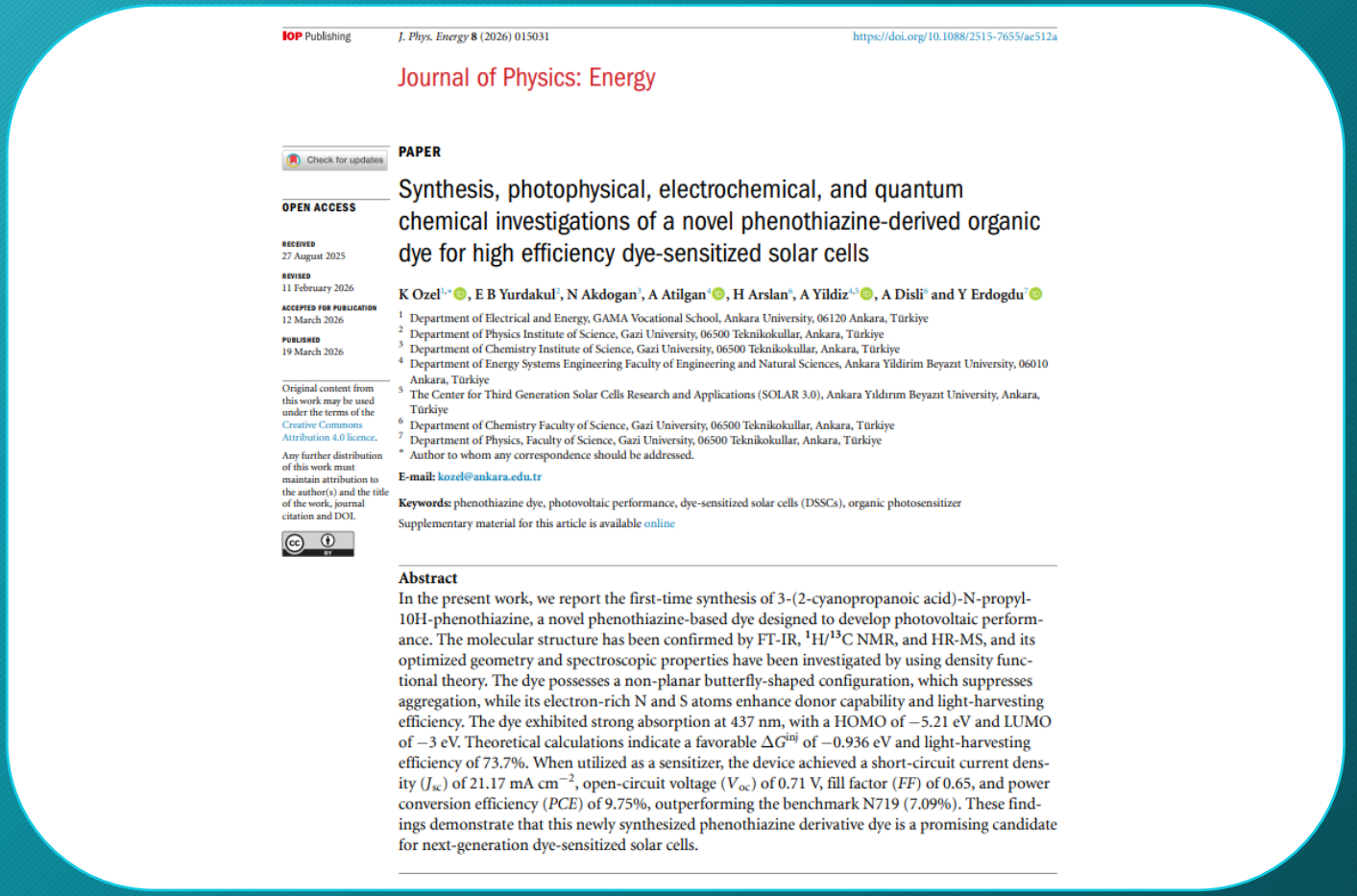

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Journal of Physics: Energy

PAPER

Synthesis, photophysical, electrochemical, and quantum chemical investigations of a novel phenothiazine-derived organic dye for high efficiency dye-sensitized solar cells

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Keywords: phenothiazine dye, photovoltaic performance, dye-sensitized solar cells (DSSCs), organic photosensitizer

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Abstract

In the present work, we report the first-time synthesis of 3-(2-cyanopropanoic acid)-N-propyl-10H-phenothiazine, a novel phenothiazine-based dye designed to develop photovoltaic performance. The molecular structure has been confirmed by FT-IR, $^{1}H/^{13}C$ NMR, and HR-MS, and its optimized geometry and spectroscopic properties have been investigated by using density functional theory. The dye possesses a non-planar butterfly-shaped configuration, which suppresses aggregation, while its electron-rich N and S atoms enhance donor capability and light-harvesting efficiency. The dye exhibited strong absorption at 437 nm, with a HOMO of −5.21 eV and LUMO of −3 eV. Theoretical calculations indicate a favorable ΔG^{inj} of −0.936 eV and light-harvesting efficiency of 73.7%. When utilized as a sensitizer, the device achieved a short-circuit current density (J_{sc}) of 21.17 mA cm^{-2}, open-circuit voltage (V_{oc}) of 0.71 V, fill factor (*FF*) of 0.65, and power conversion efficiency (*PCE*) of 9.75%, outperforming the benchmark N719 (7.09%). These findings demonstrate that this newly synthesized phenothiazine derivative dye is a promising candidate for next-generation dye-sensitized solar cells.

Waqas Siddique Subhani, M Bilal Faheem, Abdullah Atilgan, Kenan Ozel, Bilawal Khan, Madan Saud, Ashok Thapa, Yuchen Zhang, Mohsin Shahbaz, ***Abdullah Yildiz***, Quinn Qiao

Surface engineered wide-bandgap all-inorganic perovskite solar cells achieve a fill factor exceeding 82%

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Communication

Surface engineered wide-bandgap all-inorganic perovskite solar cells achieve a fill factor exceeding 82%

Waqas Siddique Subhani,[a,1] M. Bilal Faheem,[b,1*] Abdullah Atilgan,[c,d] Kenan Ozel,[c,d] Bilawal Khan,[e] Madan Saud,[b] Ashok Thapa,[b] Yuchen Zhang,[b] Mohsin Shahbaz,[f] Abdullah Yildiz,[c,d*] Quinn Qiao[b*]

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Abstract

Cesium lead iodide bromide ($CsPbIBr_2$) perovskite solar cells (PSCs) exhibit enhanced stability compared to other inorganic perovskite compositions. However, their photovoltaic performance remains a major challenge, limiting their power conversion efficiencies (PCEs). This study introduces an innovative device design aimed at improving the surface potential of $CsPbIBr_2$ PSCs by enhancing their optoelectronic properties. The method of deploying a thin layer of tetraphenyl-porphine zinc (TPP-Zn) over perovskite active layer not only suppressed surface residues and defects but also facilitated smoother charge carrier dynamics within the photovoltaic device. Interaction between TPP-Zn and the uncoordinated metal cations of $CsPbIBr_2$ perovskite effectively passivates the surface trap states of the film, resulting in enhanced charge transport and suppression of charge recombination. We further devised a solar cell model using SCAPS-1D to

Huda A Al-Ghamdi, Reda M El-Shishtawy, Abdullah M Asiri, Kenan Ozel, Abdullah Atilgan, ***Abdullah Yildiz***

Dual Donor-π-Acceptor Phenoxazine Dyes for Efficient Dye-Sensitized Solar Cells

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RESEARCH ARTICLE

Dual Donor-π-Acceptor Phenoxazine Dyes for Efficient Dye-Sensitized Solar Cells

Huda A. Al-Ghamdi[1] | Reda M. El-Shishtawy[2] | Abdullah M. Asiri[2] | Kenan Ozel[3,4] | Abdullah Atilgan[4,5] | Abdullah Yildiz[4,6]

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Keywords: cyanoacrylic acid anchor | D–D–π–A dye | dye-sensitized solar cells (DSSCs) | intramolecular charge transfer (ICT) band | phenoxazine donor

ABSTRACT

A novel D–D–π–A dye (TPC) based on a phenoxazine core and a p-tolyl auxiliary donor was designed and synthesized. The dye exhibits strong visible-light absorption, efficient intramolecular charge transfer, and promising performance when applied in dye-sensitized solar cells (DSSCs). TPC achieved a notable power conversion efficiency (PCE), demonstrating its potential as a high-efficiency organic sensitizer. When incorporated into DSSCs, the TPC dye exhibited a short-circuit current density (J_{sc}) of 19.01 mA cm^{-2}, an open-circuit voltage (V_{oc}) of 0.65 V, a fill factor (FF) of 0.62, and a PCE of 7.69% under standard AM 1.5G illumination.

H Ot, B Akaoglu, ***ABDULLAH Yildiz***

Tuning carrier transport and optical properties of Co3O4 thin films via sputtering power

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Tuning carrier transport and optical properties of Co_3O_4 thin films via sputtering power

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ARTICLE INFO

Keywords:
Sputtering power
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Thin films

ABSTRACT

This work systematically investigates the influence of sputtering power (125–225 W) on the structural, electrical, and optical properties of Co_3O_4 thin films. Room-temperature conductivity exhibits a nonlinear dependence on power, reaching its maximum at 150 W ($6.83 \times 10^{-4}\ \Omega^{-1}\cdot cm^{-1}$) and decreasing at both lower and higher powers (e.g., 225 W: $1.93 \times 10^{-4}\ \Omega^{-1}\cdot cm^{-1}$). Optimal performance is achieved at 150–200 W due to a favorable balance between crystallinity and defect density. Measurements that depend on temperature indicate two modes of conduction: non-adiabatic small polaron hopping (SPH) at elevated temperatures (with activation energies ranging from 0.059 to 0.077 eV) and three-dimensional Mott variable-range hopping (VRH) occurring below 260 K, with a transition observed between 180 and 270 K. These findings underscore the significance of intrinsic polaronic transport in applications such as catalysis, energy storage, and sensing. Optical measurements reveal two direct transitions: a weakly power-dependent ligand-field (d–d) transition at E_{g1}~1.24–1.35 eV and a ligand-to-metal charge-transfer at E_{g2}~1.76–2.20 eV. For 125–200 W, E_{g2} linearly increases with oxygen content, indicating a progressively sharper absorption onset. The 225 W film, while exhibiting the lowest oxygen content and reduced conductivity, shows the largest E_{g2}. It also shows the most pronounced spinel phase, consistent with high-power growth that densifies the film and strengthens preferred orientation. These results suggest that the apparent optical gap is governed primarily by absorption-edge sharpness and microstructure, rather than Co/O ratio alone.

ME Yelkovan, M Erdogdu, MU Özbek, Y Erdogdu, ***ABDULLAH Yildiz***

Mechanistic correlation between electron injection, recombination, and photovoltage in cota tinctoria, punica granatum, and linaria grandiflora-based natural dye-sensitized solar cells

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Mechanistic correlation between electron injection, recombination, and photovoltage in *cota tinctoria*, *punica granatum*, and *linaria grandiflora*-based natural dye-sensitized solar cells

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Keywords: dye-sensitized solar cells, natural dyes, energy-level alignment, electron injection driving force, recombination resistance, photovoltaic performance

Abstract

Natural dye-sensitized solar cells (*n*-DSSCs) offer a sustainable and low-cost alternative to conventional photovoltaics. Three natural dyes - *Cota tinctoria* (*CTT*), *Punica granatum* (*PG*), and *Linaria grandiflora* (*LG*) - are investigated as a new eco-friendly sensitizer, and their photovoltaic performance is systematically correlated with energetic parameters. Comprehensive FT-IR, UV–vis, cyclic voltammetry (CV), and electrochemical impedance spectroscopy (EIS) analyses were employed to evaluate the relationships between electron injection driving force (ΔG_{inj}), recombination resistance (R_{rec}), and open-circuit voltage (V_{OC}). Among the investigated natural dyes, the *CTT*-based device obtained the highest short-circuit current density ($J_{SC} = 2.11$ mA cm^{-2}), open-circuit voltage ($V_{OC} = 610$ mV), and efficiency ($\eta = 0.91\%$). The correlation identified between ΔG_{inj}, R_{rec}, and V_{OC} indicates that injection and recombination energies determine the efficiency of devices. These insights establish a mechanistic framework linking molecular energy alignment with photovoltaic behavior and guide the design of next-generation bio-derived sensitizers. Importantly, the study shows that superior ΔG_{inj} facilitates stronger electron injection into TiO_2, while higher R_{rec} values suppress interfacial recombination, collectively governing V_{OC} and overall efficiency. Overall, the results demonstrate that interplay between ΔG_{inj} and R_{rec} governs the photovoltaic behavior of natural dye-based DSSCs, establishing *Cota tinctoria* as a particularly promising bio-derived sensitizer for next-generation solar energy applications.

Mustafa Kurban, Beyza Furtana Yalcin, Mehmet Yilmaz, Sinan Akpinar, Baha Vural Kök, Seda Hekim, Ahmet Münir Özdemir, Erkut Yalcin, ***Fahrettin Göktaş***

Integrating experimental and atomistic insights into the rejuvenation of aged binder using bio-based rejuvenators

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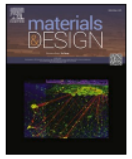

Integrating experimental and atomistic insights into the rejuvenation of aged binder using bio-based rejuvenators

Mustafa Kurban [a,*], Beyza Furtana Yalcin [b], Mehmet Yilmaz [c], Sinan Akpinar [d], Baha Vural Kök [b], Seda Hekim [c], Ahmet Münir Özdemir [e], Erkut Yalcin [b], Fahrettin Göktaş [d]

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ARTICLE INFO

Keywords:
Bio-based rejuvenator
Aged asphalt binder
Molecular dynamics (MD)
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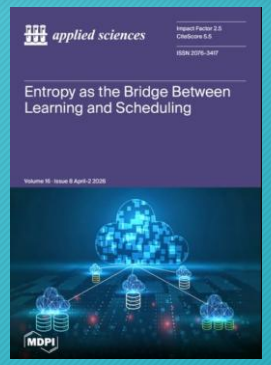
Reclaimed asphalt pavement (RAP)

ABSTRACT

This study integrates experimental and computational methods to evaluate the rejuvenation performance of an aged asphalt binder using two novel bio-based additives, 1T and 2T. The aged binder, sourced from reclaimed asphalt pavement (RAP), was modified with 25 wt% of each rejuvenator (denoted as 1T25 and 2T25, respectively). SARA (Saturates, Aromatics, Resins, Asphaltenes) fractionation and colloidal indices were used to assess compositional recovery. Both additives increased aromatic and resin contents while reducing asphaltenes. The 2T-modified binder achieved the highest colloidal stability ($I_c = 0.29$) and the most pronounced improvement in stability indicators (CI and I_c) among the tested systems. Complementary molecular dynamics (MD) simulations using the COMPASSII force field modeled the structural and thermodynamic behavior of RAP and rejuvenated systems. The 2T25 system exhibited higher density and more compact molecular packing, suggesting stronger cohesive organization and reduced free volume, whereas 1T25 showed greater molecular spacing and flexibility. RDF analysis and converged thermodynamic/structural trajectories (energy, temperature, cell length, and density stabilization) further supported rejuvenator-dependent rearrangement of packing during equilibration. Overall, MD acts as a mechanistic bridge that interprets experimental SARA/CI/I_c trends and supports design-oriented development of sustainable rejuvenators.

Endiz Mustafa Sacid, Atıl Emre Coşgun, Demir Hasan, ***Mehmet Zahid Erel***, Çalıkuşu İsmail, Elif Bahar Kılınç, Taş Aslı, Keten Gökkuş Mualla, Gökkuş Göksel

Renewable Energy Applications Across Engineering Disciplines: A Comprehensive Review



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Energy Systems Engineering

Review

Renewable Energy Applications Across Engineering Disciplines: A Comprehensive Review

Mustafa Sacid Endiz [1], Atıl Emre Coşgun [2,*], Hasan Demir [2], Mehmet Zahid Erel [3], İsmail Çalıkuşu [4], Elif Bahar Kılınç [5], Aslı Taş [6], Mualla Keten Gökkuş [6] and Göksel Gökkuş [6]

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Abstract

Renewable energy technologies are becoming more and more relevant in a variety of engineering fields as a result of the move toward low-carbon, sustainable energy systems. Although research has historically concentrated on power generation, it now covers a broad range of applications, including precision agriculture, smart grids, energy storage, healthcare devices, and sustainable buildings. However, existing review studies are often limited to single disciplines or specific technologies, lacking a unified cross-disciplinary perspective that captures the interconnected nature of modern renewable energy systems. This gap motivates the need for a comprehensive review that bridges multiple engineering domains. This review provides a comprehensive synthesis of literature on renewable energy applications in electrical and electronics, computer, environmental, biomedical, architectural, and agricultural engineering. In electrical and electronics engineering, the use of renewable energy sources is largely based on the efficient generation of electricity from natural resources such as solar, wind, and ocean energy. Computer engineering contributes through artificial intelligence (AI), Internet of Things (IoT) architectures, digital twins, and cybersecurity solutions, optimizing energy management. Environmental engineering emphasizes life cycle assessment, carbon footprint reduction, and circular economy strategies. In biomedical engineering, energy harvesting and self-powered devices illustrate micro-scale applications of renewable energy. Architectural engineering integrates renewable systems through building-integrated photovoltaics, net-zero energy designs, and smart building management, while agricultural engineering uses solar-powered irrigation, biomass utilization, agrivoltaic systems, and other sustainable practices. To support a low-carbon future with integrated and sustainable engineering solutions, this study not only highlights innovations within individual fields but also showcases how different disciplines can connect and work together. Overall, the review offers a novel cross-disciplinary framework that advances the understanding of renewable energy systems beyond isolated applications and provides direction for future integrative research.

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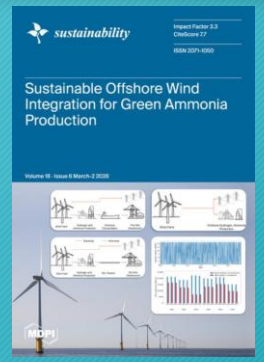
Mehmet Zahid Erel

Advanced Control of a Thermoelectric Generator-Supplied Modified Z-Source Converter for High-Gain DC Microgrids



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Article

Advanced Control of a Thermoelectric Generator-Supplied Modified Z-Source Converter for High-Gain DC Microgrids

Mehmet Zahid Erel

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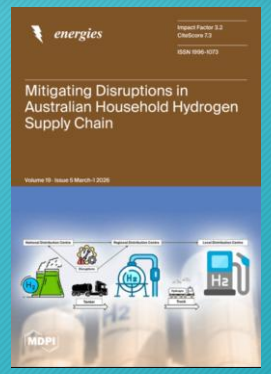
Abstract

Thermoelectric generators (TEGs) enable compact waste-heat energy harvesting but require high-gain DC–DC conversion due to their low-output voltage for DC microgrid interfacing. This work proposes a novel TEG-supplied two-stage architecture consisting of a perturb-and-observe (P&O)-based MPPT boost converter followed by a modified Z-source converter regulated through an advanced model predictive control (MPC) framework. The modified Z-source topology enables high-voltage gain without extreme duty ratios and mitigates switching losses by eliminating diode reverse-recovery effects via synchronous operation. To enhance dynamic performance, the advanced MPC strategy incorporating an adaptive ripple-based weighting mechanism is applied to the modified Z-source converter and benchmarked against MPC and sliding mode control (SMC). Simulation results under multiple disturbance scenarios, including hot-side and cold-side temperature variations, multi-condition disturbances, coupling-factor variation, and measurement noise, demonstrate that the proposed system maintains stable 400 V regulation at a 100 W output level. In contrast, MPC exhibits switching frequency deviations that increase switching losses during transient operation, while SMC suffers from significant voltage deviations under source variations. The proposed strategy maintains tight voltage regulation with nearly fixed-frequency operation around 50 kHz, providing a new perspective for TEG researchers while supporting sustainable waste-heat energy utilization.

Keywords: thermoelectric generator; waste-heat recovery; sustainable energy; modified z-source converter; advanced control; high-gain; DC microgrid

Hajer Faris, ***Musaria Karim Mahmood***, Nawal Rai, Saleh Al Dawsari, Khalid Yahya

A Hybrid Shuffled Frog Leaping–Shuffled Complex Evolution Algorithm for Photovoltaic Parameter Identification



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Article

A Hybrid Shuffled Frog Leaping–Shuffled Complex Evolution Algorithm for Photovoltaic Parameter Identification

Hajer Faris [1], Musaria Karim Mahmood [1], Nawal Rai [2], Saleh Al Dawsari [3,4,*] and Khalid Yahya [5,*]

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Abstract

Accurate identification of photovoltaic (PV) cell and module parameters remains a fundamental yet challenging task, particularly as model complexity increases from five to nine unknown parameters. In this study, the parameter extraction problem is rigorously formulated as a nonlinear optimization task and addressed using a novel hybrid metaheuristic algorithm, termed the Shuffled Frog Leaping–Shuffled Complex Evolution (SFL-SCE) method. The proposed approach synergistically integrates the population-based social learning mechanism of the Shuffled Frog Leaping Algorithm (SFL) with the robust global search and refinement capabilities of Shuffled Complex Evolution (SCE), thereby achieving an effective balance between exploration and exploitation. The SFL-SCE algorithm minimizes the root-mean-square error (RMSE) between measured and simulated current–voltage characteristics and is systematically applied to three widely used PV technologies: the RTC-France silicon solar cell, the polycrystalline Photowatt-PWP201 module, and the monocrystalline STM6-40/36 module. For each device, parameter identification is performed under one-diode, two-diode, and three-diode modelling frameworks, encompassing increasing levels of physical fidelity and computational complexity. Experimental data are employed throughout to ensure practical relevance and robustness. The performance of the proposed algorithm is comprehensively evaluated against its constituent algorithms (SFLA and SCE) as well as several state-of-the-art hybrid optimization techniques reported in the literature. Comparative results demonstrate that SFL-SCE consistently achieves superior accuracy, enhanced reliability, and faster convergence, as evidenced by lower minimum, mean, and maximum RMSE values, reduced standard deviation, and improved convergence behavior across all test cases. These findings confirm the effectiveness of the proposed hybridization strategy and establish SFL-SCE as a powerful and reliable tool for high-precision PV model parameter identification.

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Keywords: PV cell; parameter identification; shuffled frog leaping algorithm; shuffled complex evolution

Mustafa Lateef Fadhil Jumaili, Aya Abdullateef Ezat, Omer Tareq Khattab, Sulaiman M Karim, Ahmed Sedeeq Baker Al-Doori, ***Musaria Karim Mahmood***

Applying deep learning models as a tool for Alzheimer's diagnosis: An analysis using (MRI)

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Applying deep learning models as a tool for Alzheimer's diagnosis: An analysis using (MRI)

Mustafa Lateef Fadhil Jumaili; Aya Abdullateef Ezat; Omer Tareq Khattab; Sulaiman M. Karim; Ahmed Sedeeq Baker Al-Doori; Musaria Karim Mahmood

+ Author & Article Information

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Our study focuses on Alzheimer's disease (AD), a prevalent condition that impacts a significant proportion of the global population. Timely identification and accurate categorization of AD enable prompt interventions and personalized treatment. We provide an innovative and advanced automated deep learning method for early detection of AD to address this requirement. The OASIS magnetic resonance images (MRI) datasets were used from Kaggle. A total of 25,937 brain (MRI) from Alzheimer's patients and controls were used to build and validate the approach. This varied data set was carefully classified into slightly, non-demented, and very mildly demented categories. The study meticulously assesses the model's accuracy via data partitioning. Four deep learning models—InceptionV3, Mobile Net, DenseNet121 and VGG16 were tested for brain MRI image classification accuracy. The focus is on a multi-class classification task rather than binary classification, which enhances the clinical value of the model. The work includes enhanced preprocessing steps such as skull stripping, intensity normalization, and data augmentation, which helped improve the model's performance. The results showed that the VGG16 model achieved the highest accuracy of 81.32%, and performed exceptionally well in the second category, achieving an F1-score of 96.84%, highlighting the model's effectiveness in accurately distinguishing disease stages. We found that deep learning models can classify disease stages using brain MRI scans. This study contributes to the hunt for reliable AD early detection methods. We conclude that deep learning models have the ability to improve the accuracy and efficiency of diagnosis by learning from a real dataset, thus obtaining rapid treatments.

Nazime Tokgöz, ***Sıtkı Kocaoğlu***

An IMU-based dataset of falls, activities of daily living, and prayer movements (AybuFall)

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BMC Research Notes

DATA NOTE Open Access

An IMU-based dataset of falls, activities of daily living, and prayer movements (AybuFall)

Nazime Tokgöz[1] and Sıtkı Kocaoğlu[2*]

Abstract

Objectives Publicly available datasets are essential for the development, evaluation, and benchmarking of fall detection and human activity recognition algorithms. Although numerous datasets include falls and activities of daily living (ADLs), prayer movements—despite exhibiting motion patterns that may resemble falls—remain largely underrepresented. The objective of this study is to present a publicly available IMU-based dataset that explicitly includes prayer movements alongside falls and ADLs, thereby addressing an important gap in existing datasets and supporting methodological research on activity classification and false-positive reduction.

Data description The dataset comprises motion recordings of 11 types of fall movements, 13 types of activities of daily living (ADLs), and 5 types of prayer movements. Data were collected from 17 healthy young adult participants using two wearable IMU sensors placed on the forehead and forearm. Each activity was performed three times by each participant. Tri-axial accelerometer, gyroscope, and magnetometer signals were recorded at a sampling frequency of 200 Hz. All recordings were manually labeled by direct observation during data acquisition. The dataset is publicly available and systematically organized to support algorithm development, benchmarking, and reproducible research in fall detection and human activity recognition. Although data were collected from young adults, the dataset is intended as a controlled reference resource, and applicability to other populations requires further validation.

Keywords IMU dataset, Fall events, Activities of daily living (ADLs), Prayer movements, Wearable sensors, Human activity recognition

Meryem Sena Akkuş, Ceylan Bal

Katalaz Enzim Aktivite Ölçüm Yöntemleri: Literatürdeki Mevcut Yaklaşımlar, Karşılaştırmalar ve Yeni Perspektifler

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Osmaniye Korkut Ata Üniversitesi Fen Bilimleri Enstitüsü Dergisi

Osmaniye Korkut Ata University Journal of The Institute of Science and Technology

Katalaz Enzim Aktivite Ölçüm Yöntemleri: Literatürdeki Mevcut Yaklaşımlar, Karşılaştırmalar ve Yeni Perspektifler

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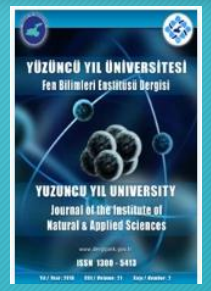
ÖZ

Katalaz enzimi, hidrojen peroksidi su ve oksijene parçalayarak oksidatif stresi düzenleyen kritik bir antioksidan enzimdir. Memeliler, bitkiler ve aerobik organizmalarda yaygın olarak bulunur ve özellikle eritrositler, karaciğer ve böbrekte yüksek konsantrasyonlarda yer alır. Tetramerik bir yapıya sahip olan katalazın NADPH bağlı formu, oksidatif inaktivasyona karşı korunmasını sağlamaktadır. Bu çalışmada, katalaz aktivitesini belirlemeye yönelik spektrofotometrik, kolorimetrik, elektroanalitik, titrimetrik, kemilüminesans ve jel bazlı yöntemler karşılaştırılmıştır. Her yöntemin avantajları, dezavantajları ve kullanım alanları detaylı şekilde değerlendirilmiş, daha hassas ve güvenilir ölçüm teknikleri geliştirmek için öneriler sunulmuştur. Ayrıca, yapay zeka ve makine öğrenmesi destekli analizlerin katalaz aktivitesi ölçümlerinde nasıl kullanılabileceği ele alınmıştır. Makine öğrenmesi tabanlı regresyon modellerinin büyük veri kümelerinden yararlanarak katalaz aktivitesini tahmin edebileceği ve ölçüm hassasiyetini artırabileceği öne sürülmüştür. Bu derleme, katalaz aktivite ölçüm yöntemlerinin mevcut durumunu kapsamlı bir şekilde inceleyerek gelecekteki çalışmalar için yeni perspektifler sunmaktadır.

Meryem Sena Akkuş

DFT Investigation of the Electronic and Catalytic Effects of Ni–Co–V Alloy Structures on the Theoretical Hydrolysis of $NaBH_4$



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Research Article

DFT Investigation of the Electronic and Catalytic Effects of Ni–Co–V Alloy Structures on the Theoretical Hydrolysis of $NaBH_4$

Meryem Sena AKKUŞ

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Abstract: This study presents a density functional theory (DFT) investigation of Ni–V, Co–V, and Ni–Co–V alloy clusters (Ni_7V_2, Co_8V_2, $Ni_6Co_4V_2$, and $Ni_4Co_4V_4$) toward sodium borohydride ($NaBH_4$) hydrolysis for hydrogen generation. The catalytic behavior was analyzed by comparing bare clusters and their $NaBH_4 + H_2O$ adsorbed reaction complexes. Structural optimizations reveal pronounced B–H bond elongation and metal–metal bond flexibility upon adsorption, particularly on Ni-rich surfaces. Electronic structure analyses indicate a systematic reduction in the HOMO–LUMO energy gap following $NaBH_4$ adsorption, confirming enhanced surface reactivity. Löwdin population analyses show significant charge transfer from borohydride to the metal framework, accompanied by a loss of hydride character and effective activation of hydrogen atoms. Thermodynamic calculations demonstrate that all reaction complexes are highly stable in aqueous media, with strongly negative enthalpy and Gibbs free energy values, indicating spontaneous and exergonic complex formation. Overall, Ni-rich and synergistic Ni–Co–V clusters exhibit superior electronic adaptability and structural stability, making them promising candidates for efficient $NaBH_4$ hydrolysis.

Keywords: DFT, HOMO–LUMO, $NaBH_4$ hydrolysis, Ni–Co–V alloys, Surface interactions

Meryem Sena Akkuş

Investigating the efficiency of NiFe catalysts in potassium borohydride hydrolysis for hydrogen production

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January 2026

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Full Length Article

Investigating the efficiency of NiFe catalysts in potassium borohydride hydrolysis for hydrogen production

Meryem Sena Akkus

Department of Energy Systems Engineering, Ankara Yıldırım Beyazıt University, 06010 Ankara, Turkey
Hydrogen Technologies and Energy Research Centre, Ankara Yıldırım Beyazıt University, 06010 Ankara, Turkey

ARTICLE INFO

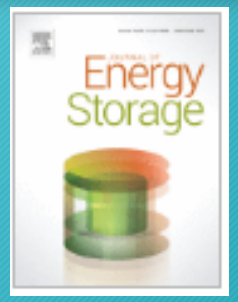
Keywords:
KBH_4
NiFe
Hydrogen production
Hydrolysis

ABSTRACT

Hydrogen production through the hydrolysis of potassium borohydride (KBH_4) is an attractive method due to its high hydrogen yield potential. This study examines the catalytic performance of a thin film nickel–iron (NiFe) catalyst in KBH_4 hydrolysis, focusing on optimizing key reaction parameters such as temperature, catalyst amount, NaOH concentration, and HCl volume. The structural and chemical properties of the NiFe catalyst were characterized using Field Emission Scanning Electron Microscopy (FESEM)/Energy Dispersive X-ray Spectroscopy (EDS), X-ray Diffraction (XRD), and Fourier Transform Infrared Spectroscopy (FTIR). The results indicate that NiFe catalysts exhibit high hydrogen production efficiency, achieving up to a 99 % yield under conditions with 1 % NaOH, 10 % KBH_4, 1.40 g catalyst, and 2.5 mL of 0.5 M HCl at 50 °C. Complementary density functional theory (DFT) calculations provided atomistic insight into the reaction mechanism, confirming the distinct roles of Fe and Ni in adsorption and electronic modulation, respectively. These combined findings demonstrate that the optimized thin film NiFe catalyst is a cost-effective and highly efficient material for hydrogen production from KBH_4, with broader implications for advanced chemical hydrogen storage technologies.

Gokhan Surucu, Cagri Karadeniz, ***Ozge Surucu***, Aysenur Gencer

Li-decorated Ti4ZnO9 monolayer for high-capacity hydrogen storage



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Research papers

Li-decorated Ti_4ZnO_9 monolayer for high-capacity hydrogen storage

Gokhan Surucu [a,*], Cagri Karadeniz [b], Ozge Surucu [c], Aysenur Gencer [d]

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[d] Department of Physics, K. O. Faculty of Science, Karamanoglu Mehmetbey University, 70200, Karaman, Türkiye

ARTICLE INFO

Keywords:
Hydrogen storage
Density functional theory
Li decoration
Ti_4ZnO_9 material

ABSTRACT

In this study, a novel two-dimensional (2D) Ti_4ZnO_9 monolayer is proposed for hydrogen storage applications, and its potential, as enhanced by Lithium (Li) decoration, was systematically investigated using first-principles density functional theory (DFT). The pristine Ti_4ZnO_9 monolayer was confirmed to be an insulator possessing robust thermodynamic, mechanical, and dynamic stability, indicating its experimental feasibility. The most energetically favorable Li decoration site (Li1) was identified, and this decoration was found to induce metallicity in the system. A significant charge transfer from the Li atoms to the Ti_4ZnO_9 surface facilitates a physisorption-based H_2 adsorption mechanism. The hydrogen storage performance of the two-sided Li1-decorated Ti_4ZnO_9 system was found to be exceptional, with a maximum gravimetric storage capacity of 6.05 wt% being achieved. This value significantly surpasses the 5.5 wt% target set by the US Department of Energy (DOE) for 2025. A critical analysis of the adsorption energies revealed the material's versatility: while the maximum 6.05 wt% capacity corresponds to a low adsorption energy (0.11 eV/H_2) suitable for cryogenic storage (85.24 K), a high capacity of 4.27 wt% is also offered. This latter capacity is achieved with an ideal adsorption energy (0.41 eV/H_2), enabling reversible storage at a near-ambient desorption temperature of 302.43 K. Based on these findings, Li-decorated Ti_4ZnO_9 is established as a highly promising and flexible platform for next-generation solid-state hydrogen storage.

Bilal Gulseven, Gokhan Surucu, ***Ozge Surucu***, Aysenur Gencer

Li-Decorated Ti2CF2 MXene for Efficient Solid-State Hydrogen Storage

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Article

Li-Decorated Ti_2CF_2 MXene for Efficient Solid-State Hydrogen Storage

Bilal Gülseven, Gokhan Surucu,* Ozge Surucu, and Aysenur Gencer

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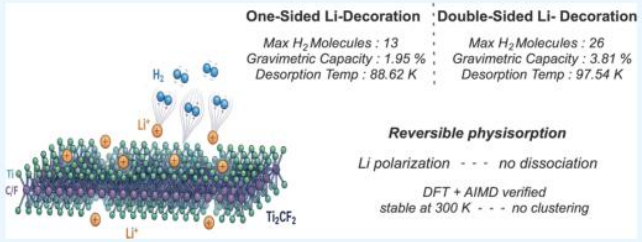

ABSTRACT: Efficient hydrogen storage is a major challenge for clean energy technologies. This study investigates the potential of Li-decorated Ti_2CF_2 MXene as a hydrogen storage material using density functional theory. Our calculations show that Li atoms bind stably to the Ti_2CF_2 surface. Ab initio molecular dynamics simulations confirm that the Li atoms do not cluster at room temperature due to strong electrostatic repulsion. The material adsorbs hydrogen molecules via a physisorption mechanism, which allows for reversible storage. It is found that double-sided Li decoration significantly improves the performance, achieving a gravimetric capacity of 3.81 wt % (26 H_2 molecules). The calculated desorption temperatures indicate that hydrogen can be released under practical conditions. These findings suggest that Li-decorated Ti_2CF_2 is a mechanically robust and dynamically stable candidate for hydrogen storage applications, offering a balanced trade-off between binding strength and reversibility.

Omer Hilal, H Gulce Emur, Anil Dogan, Elif Akhuseyin Yildiz, Mehmet Isik, Mehmet Parlak, ***Ozge Surucu***, Ayhan Elmali, Ahmet Karatay

Nonlinear optical and optical limiting properties of In2S3 chalcogenide thin films: Influence of defect states and deposition technique

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Full Length Article

Nonlinear optical and optical limiting properties of In_2S_3 chalcogenide thin films: Influence of defect states and deposition technique

Omer Hilal [a], H. Gulce Emur [a], Anil Dogan [a], Elif Akhuseyin Yildiz [b,c], Mehmet Isik [d,*], Mehmet Parlak [e], Ozge Surucu [f,g], Ayhan Elmali [b], Ahmet Karatay [b,**]

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ARTICLE INFO

Keywords:
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Optical limiting

ABSTRACT

In this study, the nonlinear absorption (NA) and optical limiting (OL) properties of indium sulfide (In_2S_3) thin films prepared by physical vapor deposition (PVD) and radio-frequency (RF) magnetron sputtering were investigated. Linear optical analysis revealed distinct Urbach energies of 1.14 eV and 0.27 eV for the PVD-grown and RF-sputtered films, respectively, indicating higher defect density in the former. Photoluminescence (PL) measurements showed broader and stronger visible emission for the RF-sputtered film, while the PVD-grown film exhibited narrower near-band-edge emission. Femtosecond transient absorption spectroscopy further revealed that the PVD-grown film featured broad excited-state absorption and faster decay dynamics, whereas the RF-sputtered film displayed ground-state bleaching and longer lifetimes, consistent with fewer traps and reduced carrier loss. Open-aperture Z-scan analysis under 532 nm, 4 ns excitation indicated intensity-dependent NA dominated by defect-assisted processes. The effective nonlinear coefficients from the defect-saturation model were over an order of magnitude higher than those from the Sheik–Bahae model. The RF-sputtered film exhibited shallower defect states that enhanced sequential two-photon and free-carrier absorption, while the PVD-grown film showed early saturation due to localized-state filling. Optical limiting thresholds of 2.63 mJ/cm^2 (RF) and 7.15 mJ/cm^2 (PVD) confirm the superior limiting performance of the RF-sputtered In_2S_3 film for visible-range nonlinear photonic applications.